

The gradient of potential vorticity, quaternions and an orthonormal frame for fluid particles

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Dedicated to Raymond Hide on the occasion of his 80th birthday.

Abstract

The gradient of potential vorticity (PV) is an important quantity because of the way PV (denoted as q) tends to accumulate locally in the oceans and atmospheres. Recent analysis by the authors has shown that the vector quantity $\mathcal{B} = \nabla q \times \nabla \theta$ for the three-dimensional incompressible rotating Euler equations evolves according to the same stretching equation as for ω the vorticity and \mathbf{B} , the magnetic field in magnetohydrodynamics (MHD). The \mathcal{B} -vector therefore acts like the vorticity ω in Euler's equations and the \mathbf{B} -field in MHD. For example, it allows various analogies, such as stretching dynamics, helicity, superhelicity and cross helicity. In addition, using quaternionic analysis, the dynamics of the \mathcal{B} -vector naturally allow the construction of an orthonormal frame attached to fluid particles; this is designated as a quaternion frame. The alignment dynamics of this frame are particularly relevant to the three-axis rotations that particles undergo as they traverse regions of a flow when the PV gradient ∇q is large.

1 Introduction

The ideas in this paper weave together two strands of research on the Euler fluid equations recently pursued by the authors. Both of these required the use of Ertel's Theorem [1] – always a favourite topic with Raymond – and were discussed at length with him during their development.

The first and latest strand of research concerns the evolution of the gradient of potential vorticity (∇q) and the gradient of potential temperature ($\nabla \theta$) [2]. In the case of the Euler equations, while both q and θ are material constants, the evolution of their gradients involves the strain and rotation rates of the flow. Physically, understanding the behaviour of ∇q in the atmosphere and the oceans is of paramount importance because potential vorticity tends to accumulate into localised spatial regions (patches) with sharp edges, where the magnitude $|\nabla q|$ is much larger than its average value [3]. In this regard, the divergenceless vector combination $\mathcal{B} = \nabla q \times \nabla \theta$ is a natural choice, because it leads to an evolution equation identical to that for either the vorticity in the incompressible three-dimensional Euler equations, or the magnetic field in an electrically conducting fluid. As a consequence, \mathcal{B} may undergo the same violent stretching and twisting associated with the vorticity field in three-dimensional turbulence, or with magnetic field lines in magnetohydrodynamics (MHD), particularly if \mathcal{B} were to align with an eigenvector of the 3×3 strain-rate matrix S associated with the fluid motion.

The second strand of research involves the use of quaternions in identifying an ortho-normal frame attached to fluid particles in an Euler flow and whose dynamics represent the tumbling of the particle as it undergoes three-dimensional rotations during its flight [4, 5]. The vector \mathcal{B} turns out to be an ideal candidate for the construction of this ortho-normal frame. This would be applicable to the dynamics of particles travelling through regions of the oceans or atmospheres which have a high values of $|\nabla q|$.

1.1 Potential vorticity gradient for the incompressible Euler

Consider the dimensionless form of the Euler equations for incompressible, stratified and rotating flow

$$\frac{D\mathbf{u}}{Dt} + 2\boldsymbol{\Omega} \times \mathbf{u} + a_0 \mathbf{k} \theta = -\nabla p, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla, \quad (1.1)$$

in which the potential temperature $\theta(\mathbf{x}, t)$ evolves passively according to

$$\frac{D\theta}{Dt} = 0. \quad (1.2)$$

In (1.1), the vectors $\boldsymbol{\Omega}$ and \mathbf{k} are the rotation rate and vertical direction, respectively, and the scalar a_0 is a dimensionless constant. Information about $\nabla \theta$ would be needed to discuss how $\theta(\mathbf{x}, t)$ might accumulate into large local concentrations. This is best studied in the context of potential vorticity defined by

$$q := \boldsymbol{\omega}_{rot} \cdot \nabla \theta \quad (1.3)$$

where $\boldsymbol{\omega}_{rot}$ is defined as $\boldsymbol{\omega}_{rot} := \boldsymbol{\omega} + 2\boldsymbol{\Omega}$ and $\boldsymbol{\omega} := \text{curl } \mathbf{u}$ denotes the fluid vorticity. Ertel's theorem says that the material time derivative D/Dt and the vector field $\boldsymbol{\omega}_{rot} \cdot \nabla$ operating

on a scalar function commute with each other under an Euler flow [1]

$$\frac{Dq}{Dt} = \left(\frac{D\boldsymbol{\omega}_{rot}}{Dt} - \boldsymbol{\omega}_{rot} \cdot \nabla \mathbf{u} \right) \cdot \nabla \theta + \boldsymbol{\omega}_{rot} \cdot \nabla \left(\frac{D\theta}{Dt} \right). \quad (1.4)$$

When $\boldsymbol{\omega}_{rot}$ obeys the incompressible Euler equations ($\nabla^\perp = (\partial_y, -\partial_x, 0)$)

$$\frac{D\boldsymbol{\omega}_{rot}}{Dt} = \boldsymbol{\omega}_{rot} \cdot \nabla \mathbf{u} - a_0 \nabla^\perp \theta \quad (1.5)$$

then q is also a material constant because

$$\frac{Dq}{Dt} = 0. \quad (1.6)$$

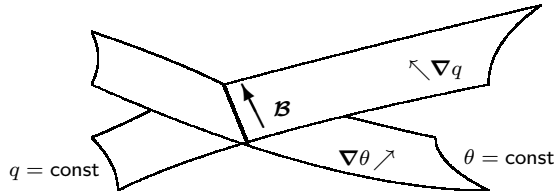


Figure 1: The vector $\mathbf{B} = \nabla q \times \nabla \theta$ is tangent to the curve defined by the intersection of the two surfaces $q = \text{const}$ and $\theta = \text{const}$ in three dimensions.

To achieve this, the following divergence-free flux vector is constructed [2]

$$\mathbf{B} = \nabla Q(q) \times \nabla \theta, \quad (1.7)$$

where $Q(q)$ is any smooth function of q . The vector \mathbf{B} , as in Figure 1, lies along the intersection of iso-surfaces of q and θ and could be thought of as pointing along the tangent to an iso-PV curve on a level set of temperature, or vice versa. Thus, the PV function $Q(q)$ is the stream function for the flux vector (\mathbf{B}) on a level set of potential temperature (θ). This observation results in the remarkably simple evolution equation

$$\frac{\partial \mathbf{B}}{\partial t} - \text{curl}(\mathbf{u} \times \mathbf{B}) = -\nabla(qQ' \text{div} \mathbf{u}) \times \nabla \theta. \quad (1.8)$$

The cross-product combination is special: an appendix in [2] contains a proof of (1.8) performed using differential geometry and also by conventional vector analysis. It follows from (1.8) that \mathbf{B} satisfies the stretching relation

$$\frac{D\mathbf{B}}{Dt} = \mathbf{B} \cdot \nabla \mathbf{u} - \mathbf{B} \text{div} \mathbf{u} - \nabla(qQ' \text{div} \mathbf{u}) \times \nabla \theta, \quad (1.9)$$

whose properties will be discussed in the next section¹.

¹In [2] the original references have been discussed ([6, 7, 8]) in which (1.8) had been derived for the incompressible Euler equations where the right hand side turned out to be zero because $\text{div} \mathbf{u} = 0$. In [2] the argument is extended to both the Navier-Stokes and hydrostatic viscous primitive equations.

1.2 Stretching, helicity, superhelicity and cross helicity

In the incompressible case where $\text{div } \mathbf{u} = 0$, equation (1.9) simplifies so that the divergenceless vector \mathbf{B} satisfies the same stretching equation as that for the vorticity $\boldsymbol{\omega}$; namely

$$\frac{D\mathbf{B}}{Dt} = \mathbf{B} \cdot \nabla \mathbf{u} \quad \text{with} \quad \text{div } \mathbf{B} = 0. \quad (1.10)$$

This leads immediately to

$$\frac{D}{Dt} |\mathbf{B}|^2 = \mathbf{B} \cdot S \mathbf{B} = \lambda^{(S)} |\mathbf{B}|^2, \quad (1.11)$$

where $\lambda^{(S)}(\mathbf{x}, t)$ is an estimate for an eigenvalue of the rate of strain matrix S and lies within its spectrum. Alignment of \mathbf{B} with a positive (negative) eigenvector of S may produce violent growth (decay) thus reproducing the stretching mechanism that produce the very large vorticity intensities that can develop locally in the early and intermediate stages of turbulence.

Moffatt's analogy between vorticity and magnetic field [9], and his detailed discussion of the topology of magnetic field lines, is based on the concept of helicity which for us requires the existence of a vector potential \mathcal{A} defined by

$$\mathcal{A} = \frac{1}{2}(Q\nabla\theta - \theta\nabla Q) + \nabla\psi, \quad (1.12)$$

in terms of the dynamical quantities Q , θ and a potential ψ . Then the helicity H , defined by

$$H = \int_V \mathcal{A} \cdot \mathbf{B} dV = \oint_{\partial V} \psi \mathbf{B} \cdot \hat{\mathbf{n}} dS, \quad (1.13)$$

measures the number of linkages of the field lines of \mathbf{B} with themselves. The time derivative of helicity under the flow of the Euler equations is given by

$$\frac{dH}{dt} = \oint_{\partial V} \left[-(\mathcal{A} \cdot \mathbf{B}) \mathbf{u} \cdot \hat{\mathbf{n}} + \left(\frac{D\psi}{Dt} \right) \mathbf{B} \cdot \hat{\mathbf{n}} \right] dS, \quad (1.14)$$

which would vanish for either homogeneous or periodic boundary conditions. For the Euler equations, $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$ is imposed on a fixed boundary. However, $H \neq 0$ and $dH/dt \neq 0$ would be possible for topography in which $\mathbf{B} \cdot \hat{\mathbf{n}} \neq 0$, so the boundaries play the only role in allowing linkages in the \mathbf{B} -field as there is no other source of helicity.

Hide's intriguing concept of a *super-helicity*, which measures the linkages of the field lines of $\mathcal{J} := \text{curl } \mathbf{B}$ with itself, may be introduced for the \mathcal{J} -vector as in for MHD [10]. Super-helicity is defined as

$$\mathcal{S} = \int_V \mathbf{B} \cdot \mathcal{J} dV. \quad (1.15)$$

After a short computation, the super-helicity dynamics for the \mathcal{J} -vector comes out to be

$$\frac{d\mathcal{S}}{dt} = \int_V 2\mathbf{B} \cdot \text{curl}^2(\mathbf{u} \times \mathbf{B}) dV + \oint_{\partial V} \left[(\mathbf{u} \cdot \mathcal{J}) \mathbf{B} \cdot \hat{\mathbf{n}} - (\mathcal{J} \cdot \mathbf{B}) \mathbf{u} \cdot \hat{\mathbf{n}} \right] dS, \quad (1.16)$$

which, unlike the helicity H , has both volume and surface sources. Likewise the *cross helicity* for the \mathbf{B} -vector can be introduced

$$\mathcal{C} = \int_V \mathbf{u} \cdot \mathbf{B} dV \quad (1.17)$$

in analogy with the corresponding quantity in MHD. Another short computation produces the dynamics of the cross helicity (\mathbf{R} is the vector potential such that $\text{curl } \mathbf{R} = 2\boldsymbol{\Omega}$)

$$\frac{d\mathcal{C}}{dt} = -a_0 \int_V (\theta \mathbf{B} \cdot \mathbf{k}) dV + \oint_{\partial V} \left(-p + \mathbf{u} \cdot \mathbf{R} + \frac{1}{2}u^2 \right) \mathbf{B} \cdot \hat{\mathbf{n}} dS, \quad (1.18)$$

which again has both volume and surface sources.

1.3 Quaternions and an attached orthonormal frame

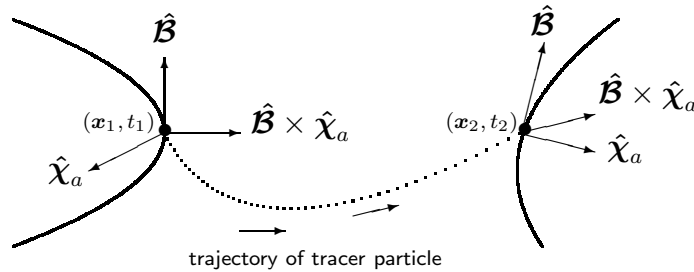


Figure 2: The solid curves represent characteristic curves $\hat{\mathbf{B}} = d\mathbf{x}/ds$ (s is arc length) to which $\hat{\mathbf{B}}$ is a unit tangent vector. The quaternion-frame orientation $(\hat{\mathbf{B}}, \hat{\mathbf{x}}_a, \hat{\mathbf{B}} \times \hat{\mathbf{x}}_a)$ is shown at the two space-time points (x_1, t_1) to (x_2, t_2) ; note that this is not the Frenet-frame corresponding to the particle path but to curves $\hat{\mathbf{B}} = d\mathbf{x}/ds$. The dotted line represents the tracer particle (\bullet) path.

More than one hundred and fifty years ago William Rowan Hamilton invented quaternions as a means of representing a composition of rotations. For most of this period they have been under-appreciated, yet they have recently undergone a spectacular renaissance due to their efficacy in certain applications in avoiding the difficulties incurred at the north and south poles² when Euler angles are used in computing the dynamics of objects undergoing three-axis rotations [11]. In particular, quaternions now lie at the heart of many modern inertial guidance systems where tracking the paths and the orientation of aircraft and satellites is of importance [12]. They are also used in the graphics community to control the orientation of tumbling objects in computer animations [11].

A natural question is whether quaternions are useful in tracking the angular velocity and orientation of Lagrangian particles in fluid dynamics. Experiments in turbulent flows have now reached the stage where the trajectories of tracer particles can be detected at high Reynolds numbers [13, 14, 15, 16]. Numerical differentiation of these trajectories gives information about the Lagrangian velocity and acceleration of the particles and also the curvature of the particle paths [16].

Conventional practice has been to consider the Frenet-frame of a trajectory. This consists of a unit tangent vector, a normal and a bi-normal, which are used to represent the pitch, yaw and roll of the motion. While the Frenet-frame describes the path, it ignores the rotational dynamics of the particle. To account for this, another ortho-normal frame associated with the

²Computations with Euler angles often suffer from “gyro-lock” because of singularities at the poles of the spherical angular coordinate system where the azimuthal angle is undefined.

motion of a Lagrangian fluid particle – designated the *quaternion-frame* – has been introduced by the authors [4]. This frame moves with the particles, but its evolution derives from the fluid equations of motion. In the context of the incompressible Euler equations, the idea of the quaternion frame depends on the existence of vectors for which there exists a Lagrangian equation of motion³. The natural triplet is $\{\boldsymbol{\omega}, \hat{\boldsymbol{\chi}}, \boldsymbol{\omega} \times \hat{\boldsymbol{\chi}}\}$ where $\boldsymbol{\chi} = \boldsymbol{\omega} \times S\boldsymbol{\omega}$ – see [4, 5]. For the incompressible Euler equations the natural candidate for the \mathcal{B} -stretching equation (1.10) is the triplet

$$\{\hat{\mathcal{B}}, \hat{\boldsymbol{\chi}}_a, \hat{\mathcal{B}} \times \hat{\boldsymbol{\chi}}_a\} \quad \text{where} \quad \boldsymbol{\chi}_a = \hat{\mathcal{B}} \times \boldsymbol{a} \quad (1.19)$$

where the \boldsymbol{a} -label has its origins in the definition $\boldsymbol{a} := \mathcal{B} \cdot \nabla \boldsymbol{u}$. The Lagrangian equations of motion for this triplet is derivable through a quaternionic formulation of the Lagrangian equation of motion for \mathcal{B} given in (1.10).

2 Quaternions, rigid body rotations and their properties

The material in this section provides the reader with a definition of quaternions, together with a précis of their multiplication rules and properties.

The literature on rotations in rigid body mechanics is replete with explicit formulae relating the Euler angles and what are called the Cayley-Klein parameters of a rotation [18]. The complicated inter-relations that are unavoidable when Euler angle formulae are used can be avoided when quaternions are used [19, 20]: for a more modern context see Holm [21, 22] and Marsden and Ratiu [23].

In terms of any scalar p and any 3-vector \boldsymbol{q} , the 4-vector quaternion $\mathfrak{q} = [p, \boldsymbol{q}]$ is defined as (Gothic fonts denote quaternions)

$$\mathfrak{q} = [p, \boldsymbol{q}] = p\mathbf{I} - \sum_{i=1}^3 q_i \sigma_i, \quad (2.1)$$

where $\{\sigma_1, \sigma_2, \sigma_3\}$ are the three Pauli spin-matrices defined by

$$\sigma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad (2.2)$$

and \mathbf{I} is the 2×2 unit matrix. A rule (denoted as \otimes) for multiplication of quaternions can be derived from the multiplication rule for the Pauli matrices $\sigma_i \sigma_j = -\delta_{ij} \mathbf{I} - \epsilon_{ijk} \sigma_k$, as

$$\mathfrak{q}_1 \otimes \mathfrak{q}_2 = [p_1 p_2 - \boldsymbol{q}_1 \cdot \boldsymbol{q}_2, p_1 \boldsymbol{q}_2 + p_2 \boldsymbol{q}_1 + \boldsymbol{q}_1 \times \boldsymbol{q}_2]. \quad (2.3)$$

Thus, the multiplication of quaternions is associative, but it is not commutative.

Let $\hat{\mathfrak{p}} = [p, \boldsymbol{q}]$ be a unit quaternion, satisfying $p^2 + q^2 = 1$. Its inverse $\hat{\mathfrak{p}}^* = [p, -\boldsymbol{q}]$ satisfies $\hat{\mathfrak{p}} \otimes \hat{\mathfrak{p}}^* = [p^2 + q^2, 0] = [1, 0]$. A pure quaternion has a zero scalar entry, such as

³The eigenvectors of the rate of strain matrix S are excluded for this reason.

$\mathfrak{r} = [0, \mathbf{r}]$. Hamilton called his pure quaternions *vectors*. Pure quaternions transform among themselves as $\mathfrak{r} = [0, \mathbf{r}] \rightarrow \mathfrak{R} = [0, \mathbf{R}]$ under

$$\mathfrak{R} = \hat{\mathbf{p}} \circledast \mathfrak{r} \circledast \hat{\mathbf{p}}^*. \quad (2.4)$$

This associative product can be written as

$$\mathfrak{R} = \hat{\mathbf{p}} \circledast \mathfrak{r} \circledast \hat{\mathbf{p}}^* = [0, (p^2 - q^2)\mathbf{r} + 2p(\mathbf{q} \times \mathbf{r}) + 2\mathbf{q}(\mathbf{r} \cdot \mathbf{q})]. \quad (2.5)$$

Choosing $p = \pm \cos \frac{1}{2}\theta$ and $\mathbf{q} = \pm \hat{\mathbf{n}} \sin \frac{1}{2}\theta$, where $\hat{\mathbf{n}}$ is the unit normal to \mathbf{r} , we find that

$$\mathfrak{R} = \hat{\mathbf{p}} \circledast \mathfrak{r} \circledast \hat{\mathbf{p}}^* = [0, \mathbf{r} \cos \theta + (\hat{\mathbf{n}} \times \mathbf{r}) \sin \theta] \equiv O(\theta, \hat{\mathbf{n}})\mathbf{r}, \quad (2.6)$$

where

$$\hat{\mathbf{p}} = \pm [\cos \frac{1}{2}\theta, \hat{\mathbf{n}} \sin \frac{1}{2}\theta]. \quad (2.7)$$

Equation (2.6) is the Euler-Rodrigues formula for the rotation $O(\theta, \hat{\mathbf{n}})$ by an angle θ of the 3-vector \mathbf{r} about its normal $\hat{\mathbf{n}}$ and the quantities $\theta, \hat{\mathbf{n}}$ are the Euler parameters. The elements of the unit quaternion $\hat{\mathbf{p}}$ are the Cayley-Klein parameters which are related to the Euler angles [18]. When $\hat{\mathbf{p}}$ is time-dependent, the Euler-Rodrigues formula in (2.6) is

$$\mathfrak{R}(t) = \hat{\mathbf{p}} \circledast \mathfrak{r} \circledast \hat{\mathbf{p}}^* \quad \Rightarrow \quad \mathfrak{r} = \hat{\mathbf{p}}^* \circledast \mathfrak{R}(t) \circledast \hat{\mathbf{p}}. \quad (2.8)$$

It is necessary to use the property of the pure quaternion $\mathfrak{R}^* = -\mathfrak{R}$ to obtain the time derivative of \mathfrak{R}

$$\dot{\mathfrak{R}}(t) = (\dot{\hat{\mathbf{p}}} \circledast \hat{\mathbf{p}}^*) \circledast \mathfrak{R} - ((\dot{\hat{\mathbf{p}}} \circledast \hat{\mathbf{p}}^*) \circledast \mathfrak{R})^*. \quad (2.9)$$

The quaternion $\hat{\mathbf{p}} = [p, \mathbf{q}]$ is of unit length and so $p\dot{p} + \mathbf{q}\dot{\mathbf{q}} = 0$, which means that $\dot{\hat{\mathbf{p}}} \circledast \hat{\mathbf{p}}^*$ is also a pure quaternion

$$\dot{\hat{\mathbf{p}}} \circledast \hat{\mathbf{p}}^* = [0, \frac{1}{2}\Omega_0(t)]. \quad (2.10)$$

The 3-vector entry in (2.10) defines the angular frequency $\Omega_0(t)$ as $\Omega_0 = 2(-\dot{p}\mathbf{q} + \dot{\mathbf{q}}p - \dot{\mathbf{q}} \times \mathbf{q})$ thereby giving the well-known formula for the rotation of a rigid body

$$\dot{\mathbf{R}} = \Omega_0 \times \mathbf{R}. \quad (2.11)$$

For a Lagrangian particle, the equivalent of Ω_0 is the Darboux vector \mathcal{D}_a in Theorem 1 in the next section.

3 An ortho-normal frame and particle trajectories

Having set the scene in §2 by describing some of the essential properties of quaternions, it is now time to apply them to the Lagrangian relation (1.10) between the two vectors \mathcal{B} and \mathcal{a}

$$\frac{D\mathcal{B}}{Dt} = \mathcal{a} := \mathcal{B} \cdot \nabla \mathbf{u}. \quad (3.1)$$

It will turn out below that a knowledge of $D\mathbf{a}/Dt$ is needed. Ertel's Theorem is applicable and the result becomes a version of Ohkitani's relation [17]

$$\frac{D}{Dt}(\mathbf{B} \cdot \nabla \mathbf{u}) = \mathbf{B} \cdot \nabla \left(\frac{D\mathbf{u}}{Dt} \right) \quad (3.2)$$

$$= -P\mathbf{B} - \mathbf{B} \cdot \nabla (2\boldsymbol{\Omega} \times \mathbf{u} + a_0 \mathbf{k}\theta) \quad (3.3)$$

where the Hessian matrix of the pressure p is defined as

$$P = \frac{\partial^2 p}{\partial x_i \partial x_j}. \quad (3.4)$$

Thus we can define a vector \mathbf{b} such that

$$\frac{D\mathbf{a}}{Dt} = \mathbf{b} := -P\mathbf{B} - \mathbf{B} \cdot \nabla (2\boldsymbol{\Omega} \times \mathbf{u} + a_0 \mathbf{k}\theta). \quad (3.5)$$

Through the multiplication rule in (2.3) quaternions appear in the decomposition of the 3-vector \mathbf{a} into parts parallel and perpendicular to another vector, which we choose to be \mathbf{B} . This decomposition is expressed as

$$\mathbf{a} = \alpha_a \mathbf{B} + \chi_a \times \mathbf{B} = [\alpha_a, \chi_a] \circledast [0, \mathbf{B}], \quad (3.6)$$

where the scalar α_a and 3-vector χ_a are defined as

$$\alpha_a = \mathcal{B}^{-1}(\hat{\mathbf{B}} \cdot \mathbf{a}), \quad \chi_a = \mathcal{B}^{-1}(\hat{\mathbf{B}} \times \mathbf{a}). \quad (3.7)$$

Equation (3.6) thus shows that the quaternionic product is summoned in naturally.⁴ It is now easily seen that α_a is the *growth rate* of the scalar magnitude ($\mathcal{B} = |\mathbf{B}|$) which obeys

$$\frac{D\mathcal{B}}{Dt} = \alpha_a \mathcal{B}, \quad (3.8)$$

while χ_a , the *swing rate* of the unit tangent vector $\hat{\mathbf{B}} = \mathbf{B}\mathcal{B}^{-1}$, satisfies

$$\frac{D\hat{\mathbf{B}}}{Dt} = \chi_a \times \hat{\mathbf{B}}. \quad (3.9)$$

Now define the two quaternions

$$\mathbf{q}_a = [\alpha_a, \chi_a], \quad \mathfrak{B} = [0, \mathbf{B}], \quad (3.10)$$

so (3.1) can automatically be re-written in the quaternion form

$$\frac{D\mathfrak{B}}{Dt} = \mathbf{q}_a \circledast \mathfrak{B}. \quad (3.11)$$

⁴With reference to §2, the Cayley-Klein parameters of the quaternion $\mathbf{q} = [\alpha, \chi]$ are

$$\hat{\mathbf{q}} = \left[\frac{\alpha}{\alpha^2 + \chi^2}, \frac{\chi}{\alpha^2 + \chi^2} \right].$$

Moreover, because of (3.5), exactly as for \mathbf{q}_a , a quaternion \mathbf{q}_b can be defined which is based on the variables

$$\alpha_b = \mathcal{B}^{-1}(\hat{\mathcal{B}} \cdot \mathbf{b}), \quad \chi_b = \mathcal{B}^{-1}(\hat{\mathcal{B}} \times \mathbf{b}), \quad (3.12)$$

where

$$\mathbf{q}_b = [\alpha_b, \chi_b]. \quad (3.13)$$

The 3-vector $\mathbf{b} = D\mathbf{a}/Dt$ admits a decomposition similar to that for \mathbf{a} as in (3.6)

$$\frac{D^2 \mathfrak{B}}{Dt^2} = [0, \mathbf{b}] = [0, \alpha_b \mathcal{B} + \chi_b \times \mathcal{B}] = \mathbf{q}_b \circledast \mathfrak{B}. \quad (3.14)$$

Using the associativity property, compatibility of (3.14) and (3.11) implies that ($\mathcal{B} = |\mathcal{B}| \neq 0$)

$$\left(\frac{D\mathbf{q}_a}{Dt} + \mathbf{q}_a \circledast \mathbf{q}_a - \mathbf{q}_b \right) \circledast \mathfrak{B} = 0. \quad (3.15)$$

This establishes a Riccati relation between \mathbf{q}_a and \mathbf{q}_b

$$\frac{D\mathbf{q}_a}{Dt} + \mathbf{q}_a \circledast \mathbf{q}_a = \mathbf{q}_b, \quad (3.16)$$

with components

$$\frac{D}{Dt}[\alpha_a, \chi_a] + [\alpha_a^2 - \chi_a^2, 2\alpha_a \chi_a] = [\alpha_b, \chi_b], \quad (3.17)$$

where $\chi_a = |\chi_a|$. There follows a Theorem on a Lagrangian particle undergoing fluid motion that is equivalent to the well-known formula (2.11) for a rigid body undergoing rotation about its center of mass:

Theorem 1 (Alignment dynamics) *The ortho-normal quaternion-frame $(\hat{\mathcal{B}}, \hat{\chi}_a, \hat{\mathcal{B}} \times \hat{\chi}_a)$ has Lagrangian time derivatives*

$$\frac{D\hat{\mathcal{B}}}{Dt} = \mathcal{D}_a \times \hat{\mathcal{B}}, \quad (3.18)$$

$$\frac{D(\hat{\mathcal{B}} \times \hat{\chi}_a)}{Dt} = \mathcal{D}_a \times (\hat{\mathcal{B}} \times \hat{\chi}_a), \quad (3.19)$$

$$\frac{D\hat{\chi}_a}{Dt} = \mathcal{D}_a \times \hat{\chi}_a, \quad (3.20)$$

where the Darboux angular velocity vector \mathcal{D}_a is defined as

$$\mathcal{D}_a = \chi_a + \frac{c_b}{\chi_a} \hat{\mathcal{B}}, \quad c_b = \hat{\mathcal{B}} \cdot (\hat{\chi}_a \times \chi_b), \quad (3.21)$$

and the quantities $[\alpha_a, \chi_a]$ and $[\alpha_b, \chi_b]$ are defined in (3.7) and (3.12).

Remark : The Darboux vector \mathcal{D}_a is driven by the 3-vector $\mathbf{b} = D\mathbf{a}/Dt$ which sits in c_b in (3.21). The analogy with rigid body rotation expressed in (2.11) is clear.

Proof: To find an expression for the Lagrangian time derivatives of the components of the frame $(\hat{\mathbf{B}}, \hat{\mathbf{x}}_a, \hat{\mathbf{B}} \times \hat{\mathbf{x}}_a)$ requires the derivative of $\hat{\mathbf{x}}_a$. To find this, it is necessary to use the fact that the 3-vector \mathbf{b} can be expressed in this ortho-normal frame as the linear combination

$$\mathcal{B}^{-1}\mathbf{b} = \alpha_b \hat{\mathbf{B}} + c_b \hat{\mathbf{x}}_a + d_b (\hat{\mathbf{B}} \times \hat{\mathbf{x}}_a). \quad (3.22)$$

where c_b is defined in (3.21) and $d_b = -(\hat{\mathbf{x}}_a \cdot \mathbf{x}_b)$. The 3-vector product $\mathbf{x}_b = \mathcal{B}^{-1}(\hat{\mathbf{B}} \times \mathbf{b})$ yields

$$\mathbf{x}_b = c_b (\hat{\mathbf{B}} \times \hat{\mathbf{x}}_a) - d_b \hat{\mathbf{x}}_a. \quad (3.23)$$

When split into components, equation (3.17) becomes

$$\frac{D\alpha_a}{Dt} = \chi_a^2 - \alpha_a^2 + \alpha_b \quad (3.24)$$

and

$$\frac{D\chi_a}{Dt} = -2\alpha_a \chi_a + \chi_b. \quad (3.25)$$

A little more working gives the *alignment dynamics* in equations (3.18)-(3.21). ■

4 Conclusions

When the quaternion approach to rotations outlined in §2 is applied to the Euler equations it demonstrates that quaternions are a natural way of calculating the orientation of Lagrangian particles in motion through the concept of ortho-normal quaternion-frames attached to each particle. In this particular context, where the \mathbf{B} -field is the vector that helps us understand the evolution of ∇q and $\nabla \theta$, knowledge of the quartet of 3-vectors $(\mathbf{u}, \mathbf{B}, \mathbf{a}, \mathbf{b})$ is sufficient for the application of Theorem 1. The complexity of the 3D Euler equations comes through the ortho-normal dynamics via the pressure field. In the present state of knowledge, the projection $P\mathbf{B}$ that is part of \mathbf{b} would have to be found by computational means.

A natural question is whether these ideas can be applied to the Navier-Stokes equations? It turns out that the evolution equation for \mathbf{B} in the incompressible case is the same as that in (1.9) with \mathbf{u} replaced by \mathbf{U} [2]. \mathbf{U} is a new transport velocity calculated using the method of Haynes and McIntyre [24]

$$q(\mathbf{U} - \mathbf{u}) = - \{ [Re^{-1} \Delta \mathbf{u} + 2\boldsymbol{\Omega} \times \mathbf{u} + a_0 \mathbf{k} \theta] \times \nabla \theta + (\sigma Re)^{-1} \boldsymbol{\omega} \Delta \theta \} \quad (4.1)$$

The quaternion procedure can only be pursued to a certain point for the Navier-Stokes equations, after which a difficulty appears when $D\mathbf{U}/Dt$ is needed, and we have no proper knowledge of this. This is consistent with the objections that \mathbf{U} is not a genuine *physical* velocity but merely a mathematical construction [25, 26]. For the Euler equations we know that this is the point where the Hessian matrix of the pressure is introduced in equation (3.2). Moreover, the stretching relation (1.9) in this case becomes

$$\frac{D\mathbf{B}}{Dt} = \mathbf{B} \cdot \nabla \mathbf{U} - \mathbf{B} \operatorname{div} \mathbf{U} - \nabla(qQ' \operatorname{div} \mathbf{U}) \times \nabla \theta, \quad (4.2)$$

and $\operatorname{div} \mathbf{U} \neq 0$, which allows richer and potentially more singular alignment dynamics than those for the incompressible case discussed here in equations (3.18)-(3.21). As well as the Navier-Stokes alluded to above, the case of the hydrostatic primitive equations have been discussed in this context in [2].

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